

Electronic Supplementary Information (ESI) for Journal of CrystEngComm.

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SUPPORTING INFORMATION

Fluorogenic Naked-Eye Sensing and Live-Cell Imaging of Cyanide by Hydrazine-Functionalized CAU-10 Metal-Organic Framework

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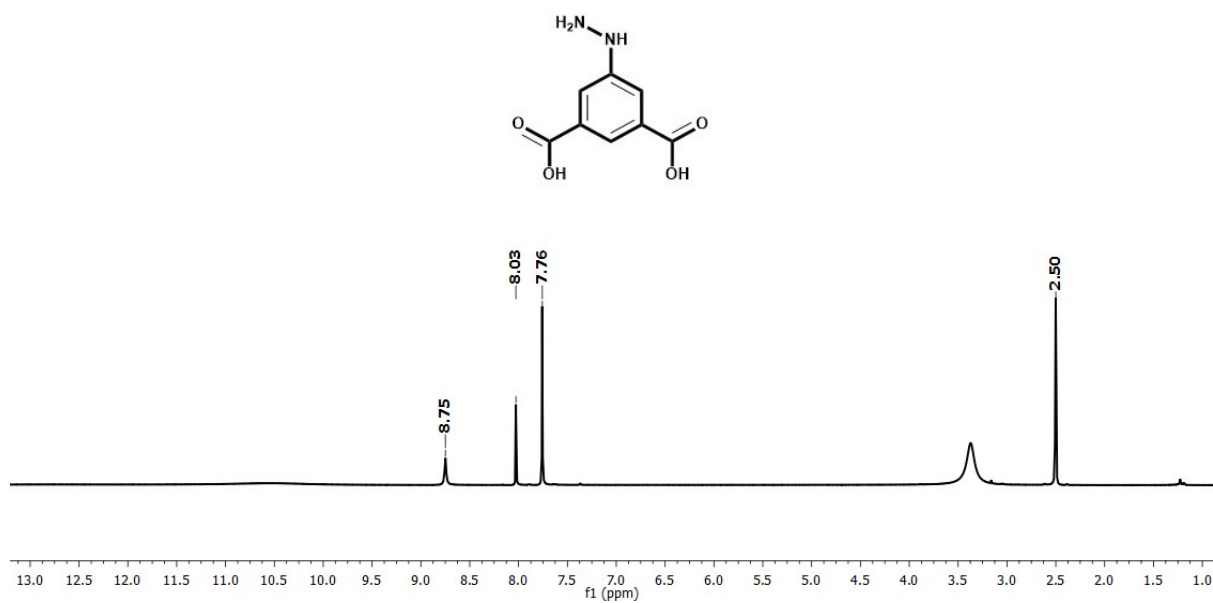


Figure S1. ^1H NMR spectrum of $\text{H}_2\text{IPA}-\text{N}_2\text{H}_3$ ligand measured in $\text{DMSO}-d_6$.

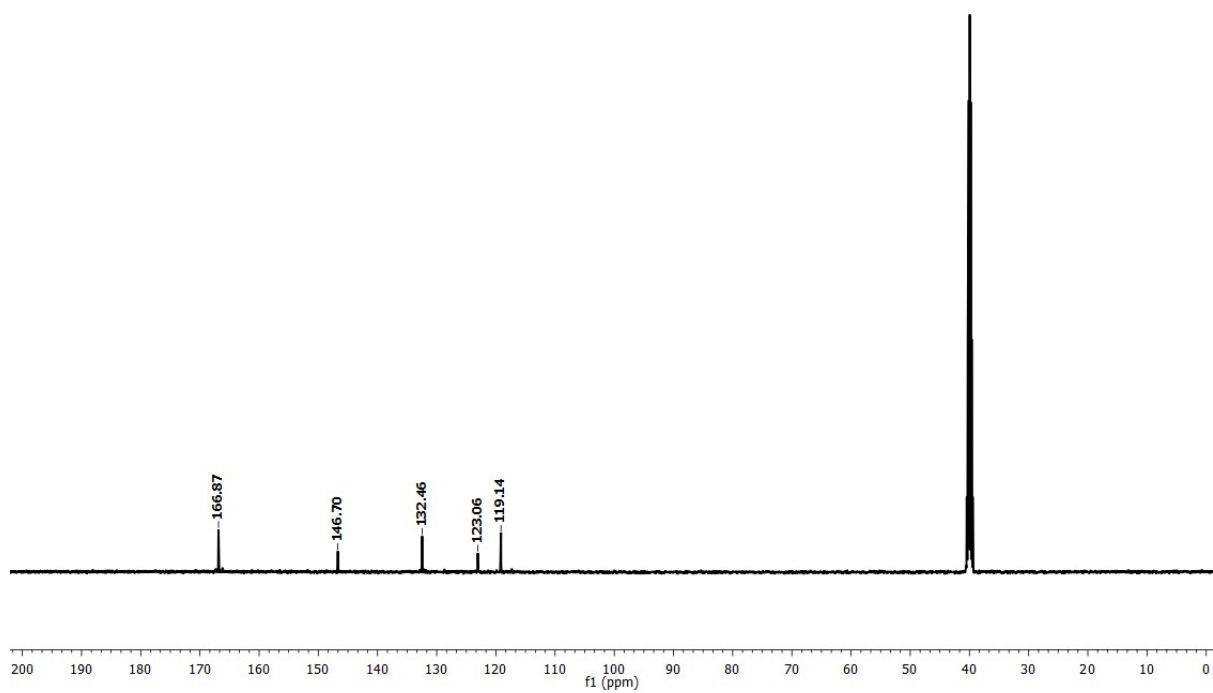


Figure S2. ^{13}C NMR spectrum of $\text{H}_2\text{IPA}-\text{N}_2\text{H}_3$ ligand measured in $\text{DMSO}-d_6$.

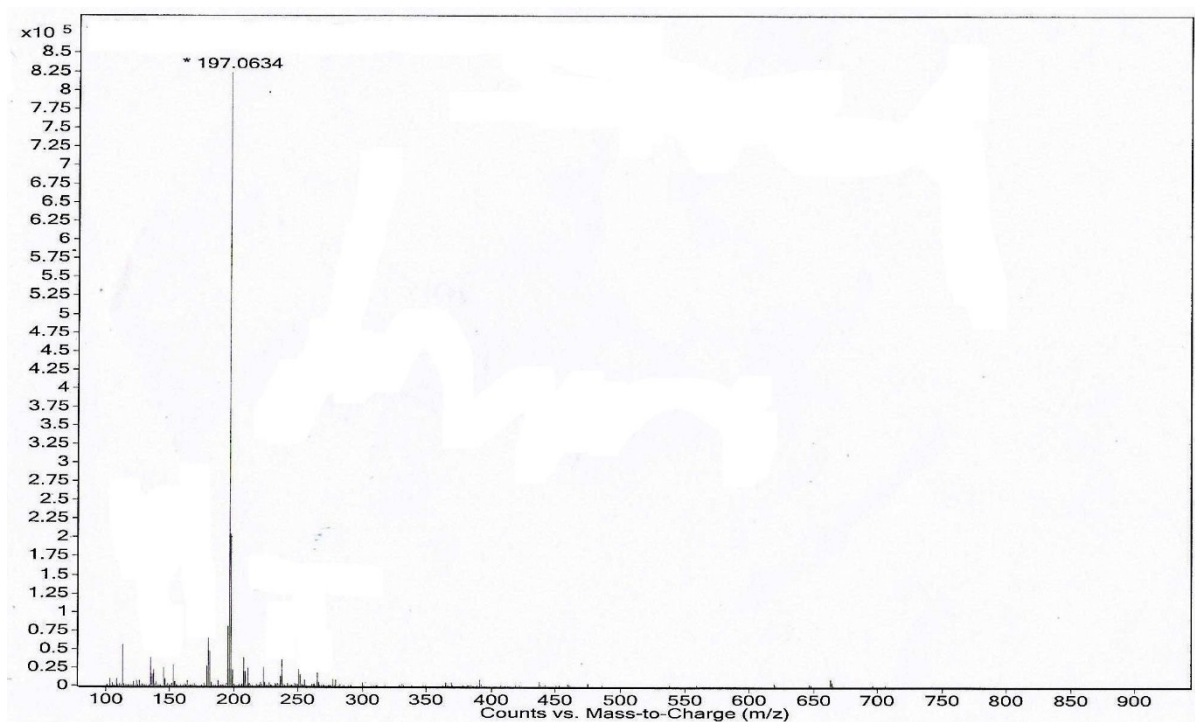


Figure S3. ESI-MS spectrum of H₂IPA-N₂H₃ ligand.

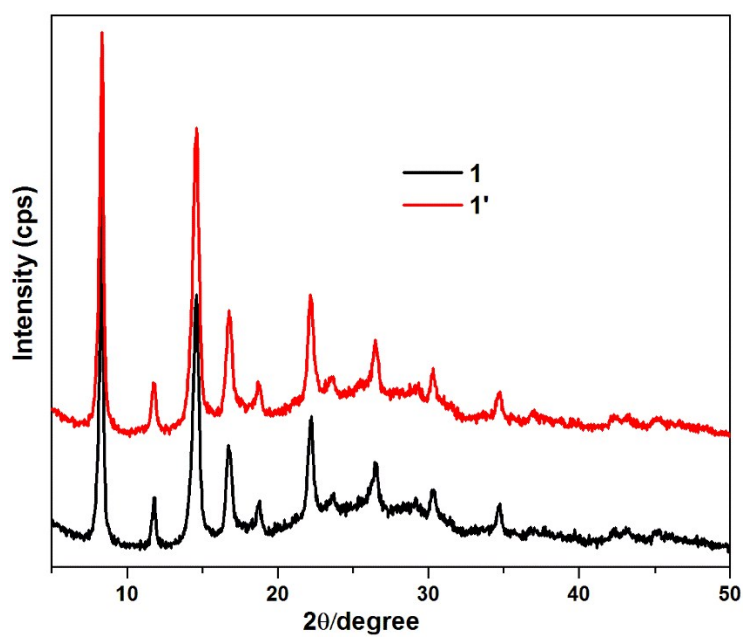


Figure S4. XRPD patterns of as-synthesized **1** and thermally activated **1'**.

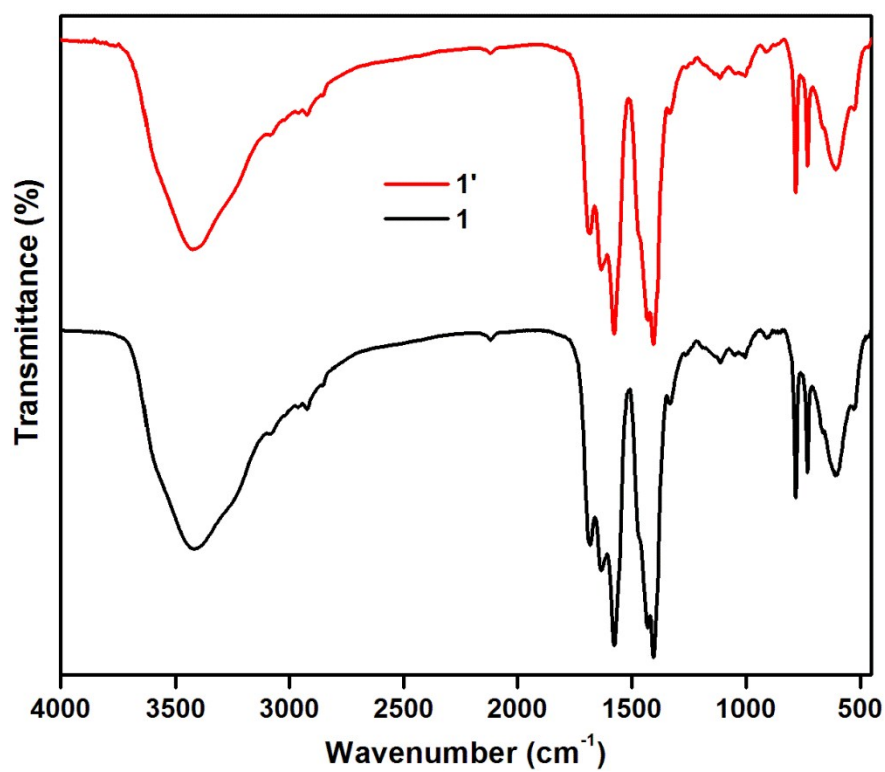


Figure S5. FT-IR spectra of as-synthesized **1** and thermally activated **1'**.

Table S1. Pawley refinement parameters for **1** and **1'**.

Compound	1	1'
space group	$I4_1/a$	$I4_1/a$
$a = b$ [Å]	21.379(16)	21.395(12)
c [Å]	11.346(8)	11.223(6)
$\alpha = \beta = \gamma$ [°]	90	90
R_{WP} [%]	3.3	3.6
GoF	2.2	2.4

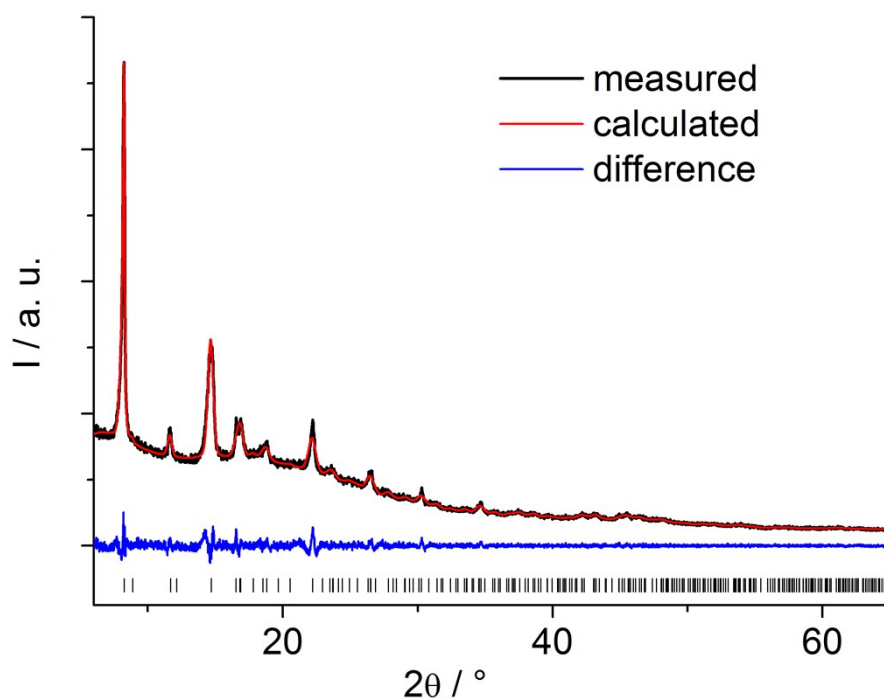


Figure S6. Final Pawley refinement plot for activated **1**. The black curve represents the measured data and the red curve is the theoretical data. The vertical black bars mark the allowed Bragg reflection positions.

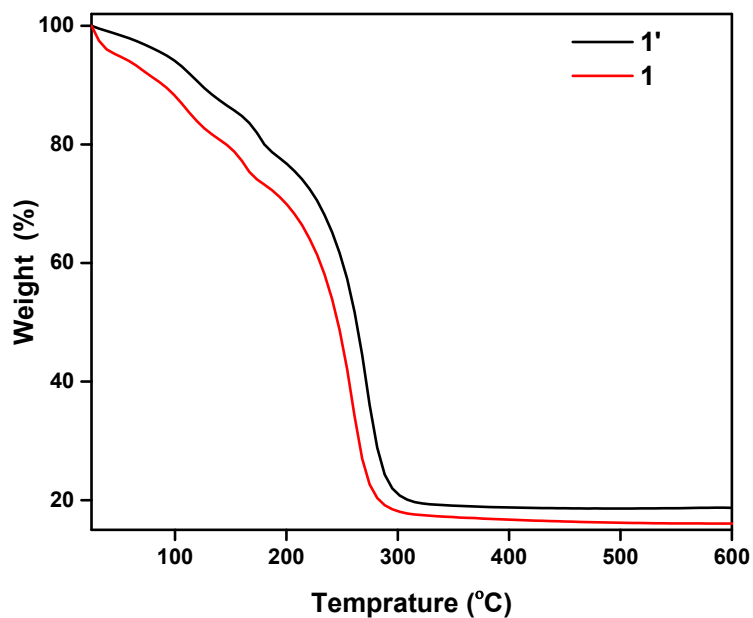


Figure S7. TG curves of **1** and **1'** recorded in an air atmosphere in the temperature range of 25-600 °C with a heating rate of 5 °C min⁻¹.

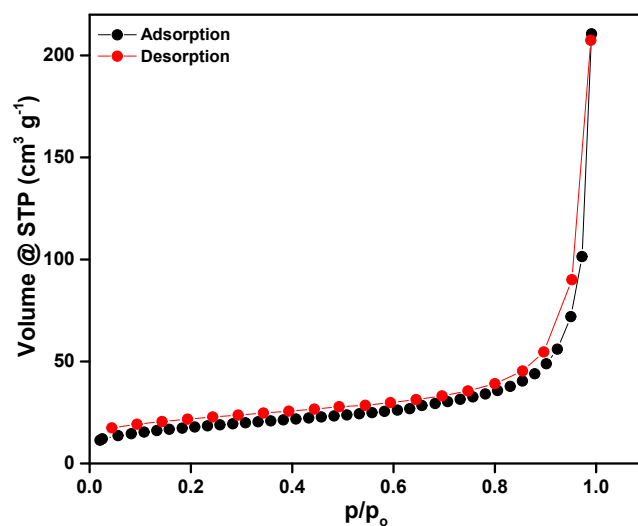


Figure S8. N₂ adsorption (black circles) and desorption (red circles) isotherms of **1'** recorded at -196 °C.

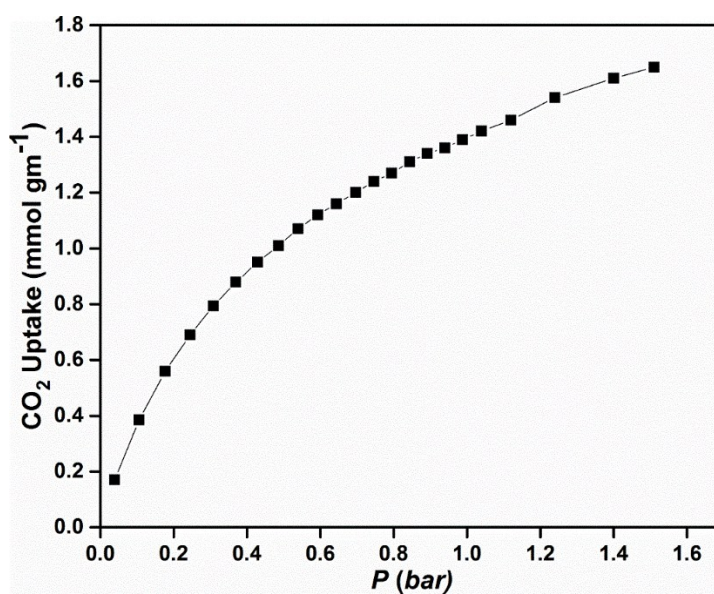


Figure S9. CO₂ adsorption of **1'** recorded at 25 °C.

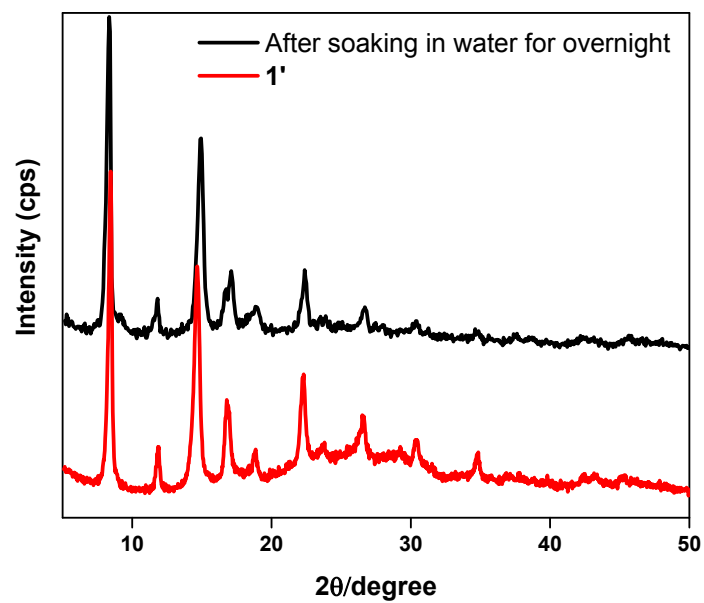


Figure S10. XRPD pattern of **1'** after soaking in water for overnight.

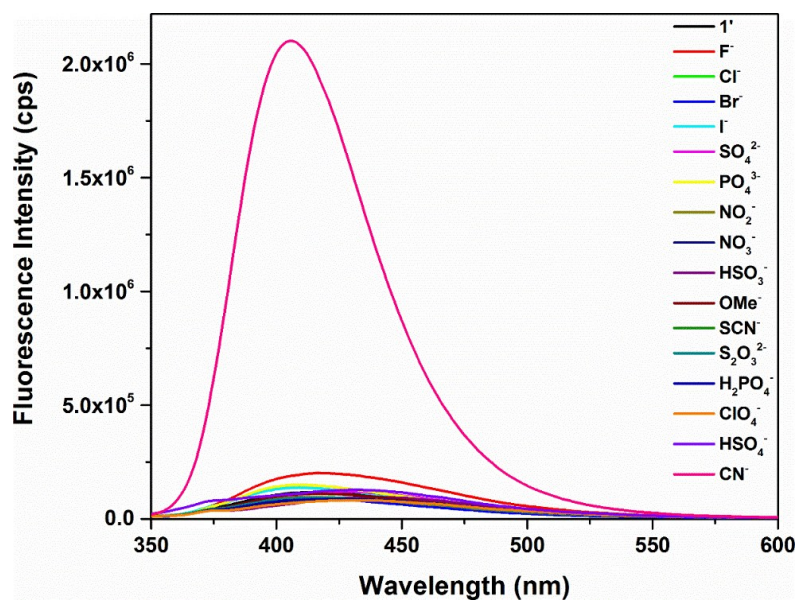


Figure S11. Change in the fluorescence intensity of **1'** upon addition of 4 mM solution (500 μ L) of various anions.

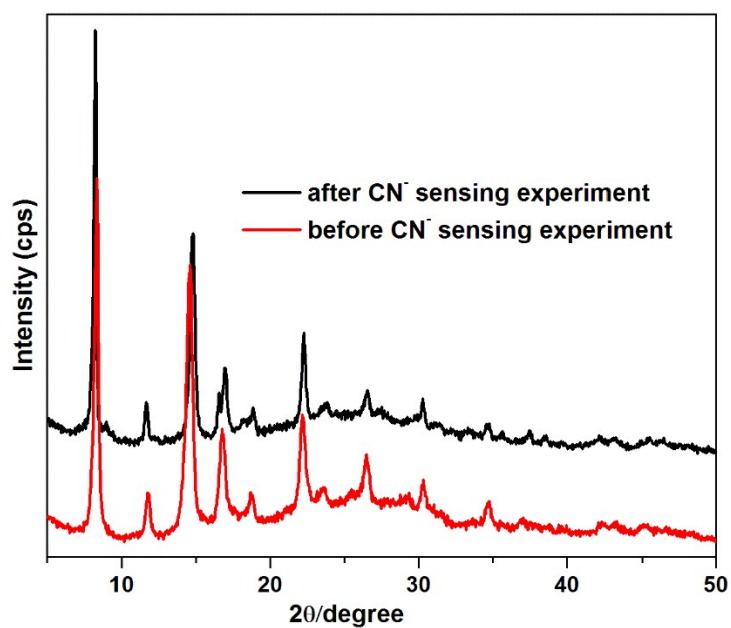


Figure S12. XRPD patterns of **1'** before and after the CN^- sensing experiment.

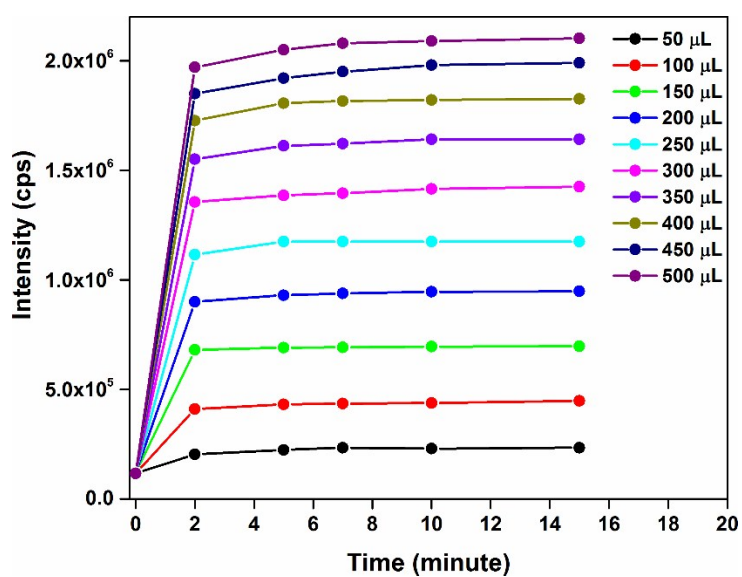


Figure S13. Time-dependent change in the fluorescence intensity of **1'** upon addition of different concentrations of CN^- ion.

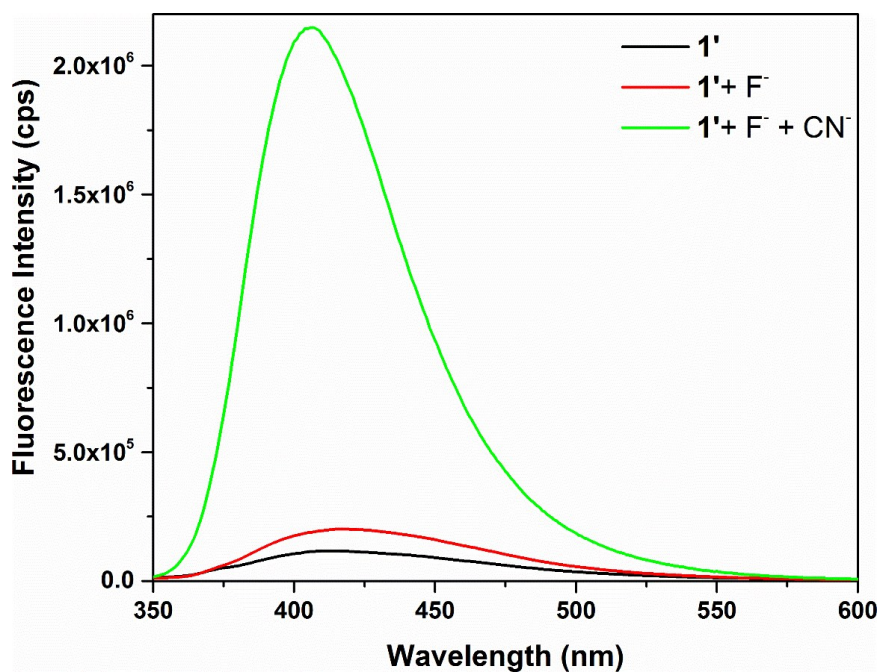


Figure S14. Change in the fluorescence intensity of **1'** upon addition of 4 mM CN⁻ solution (500 μ L) in presence of F⁻ ion (500 μ L).

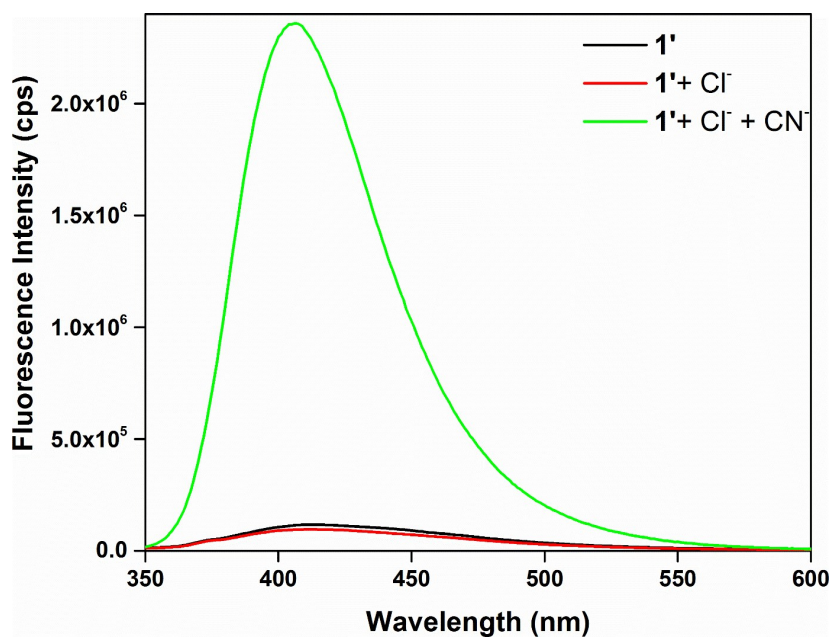


Figure S15. Change in the fluorescence intensity of **1'** upon addition of 4 mM CN⁻ solution (500 μ L) in presence of Cl⁻ ion (500 μ L).

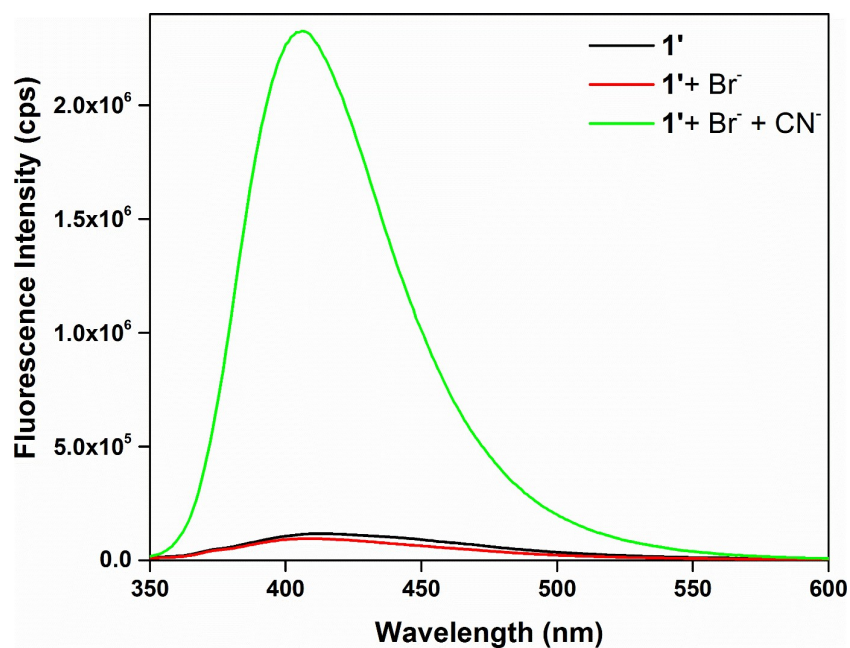


Figure S16. Change in the fluorescence intensity of **1'** upon addition of 4 mM CN⁻ solution (500 μ L) in presence of Br⁻ ion (500 μ L).

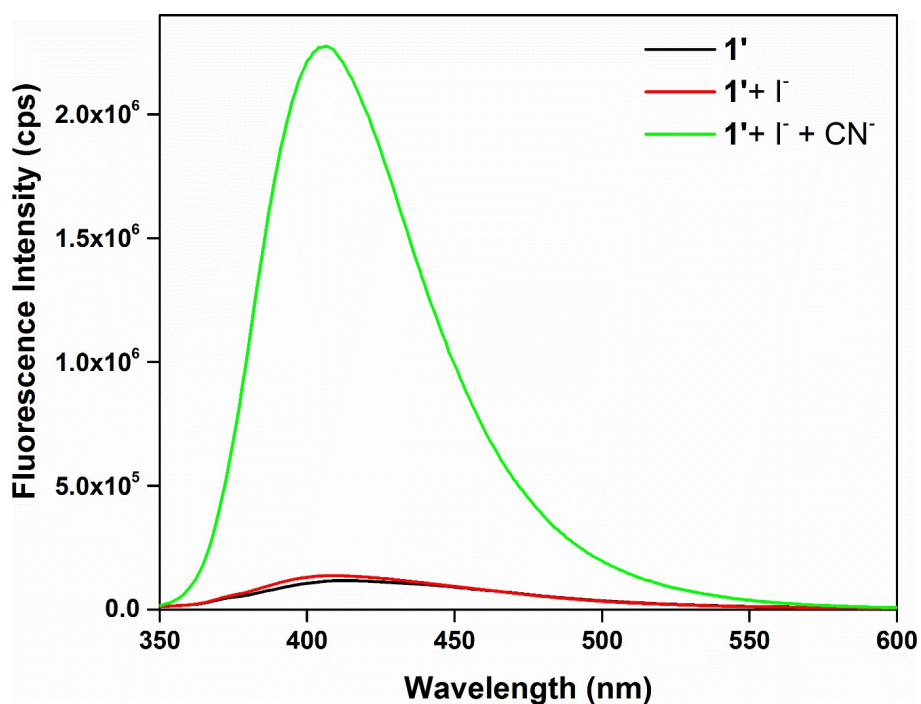


Figure S17. Change in the fluorescence intensity of **1'** upon addition of 4 mM CN⁻ solution (500 μ L) in presence of I⁻ ion (500 μ L).

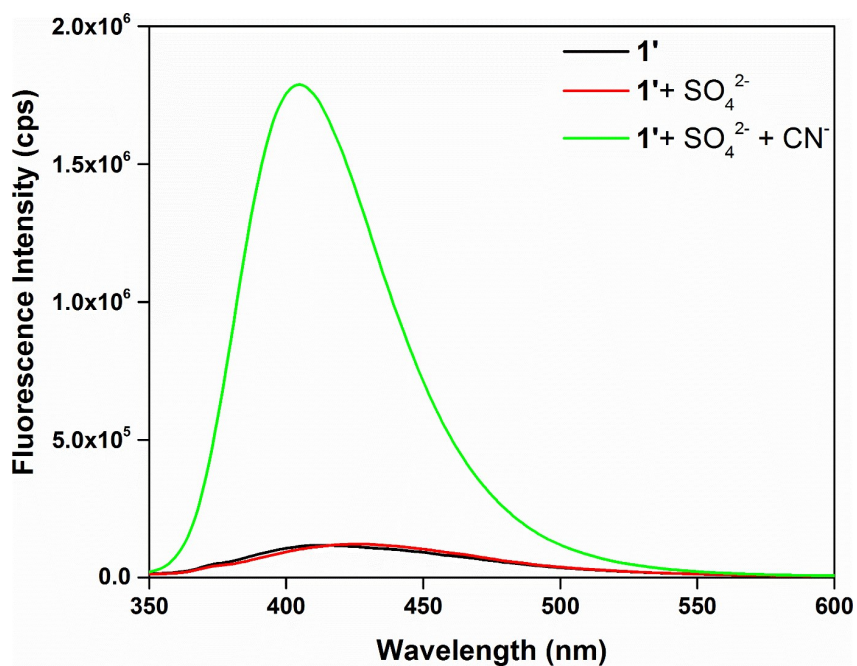


Figure S18. Change in the fluorescence intensity of **1'** upon addition of 4 mM CN^- solution (500 μL) in presence of SO_4^{2-} ion (500 μL).

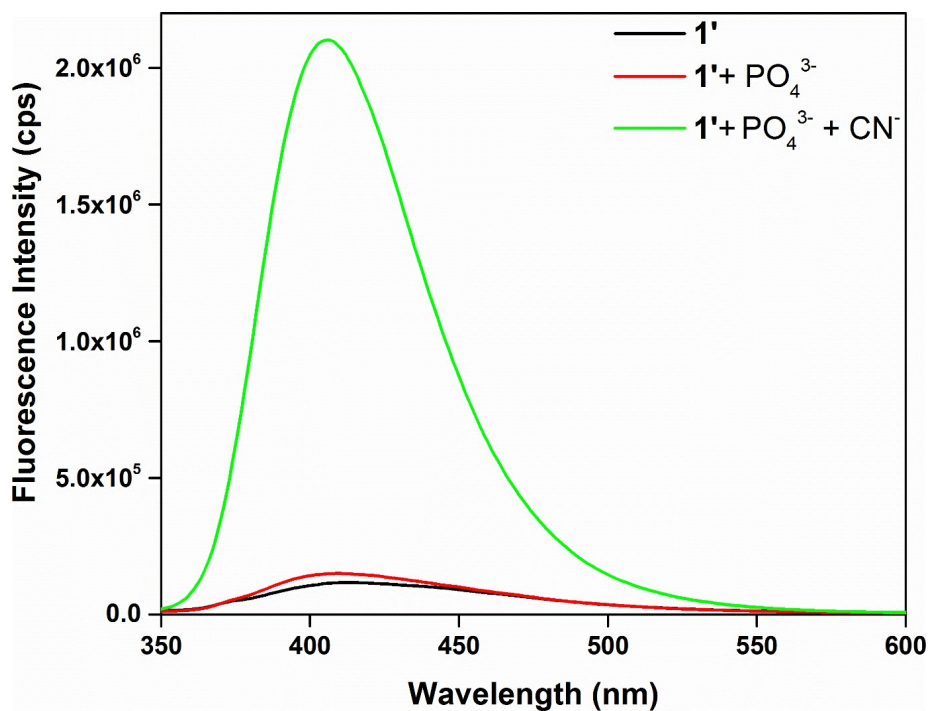


Figure S19. Change in the fluorescence intensity of **1'** upon addition of 4 mM CN^- solution (500 μL) in presence of PO_4^{3-} ion (500 μL).

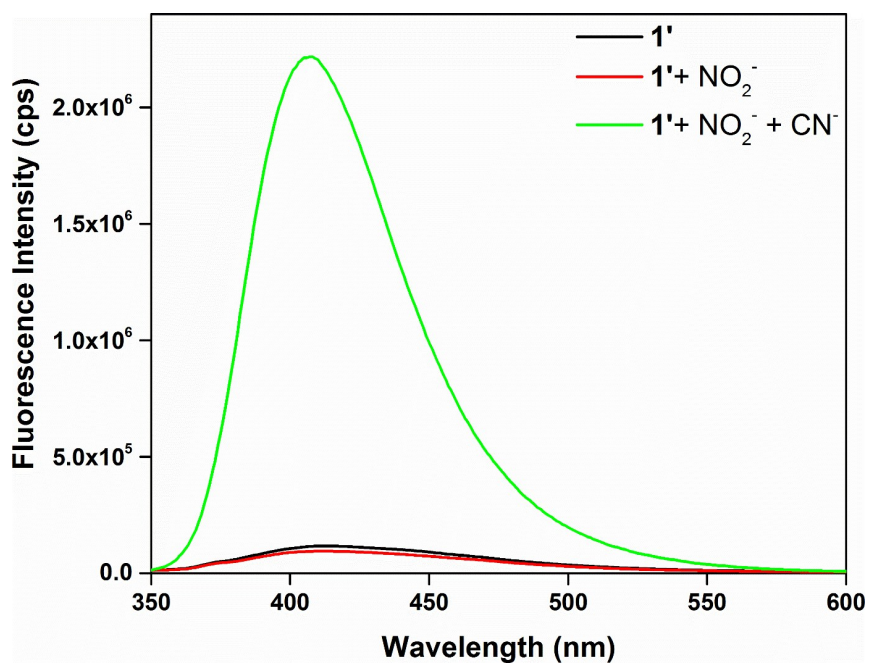


Figure S20. Change in the fluorescence intensity of **1'** upon addition of 4 mM CN⁻ solution (500 μL) in presence of NO₂⁻ ion (500 μL).

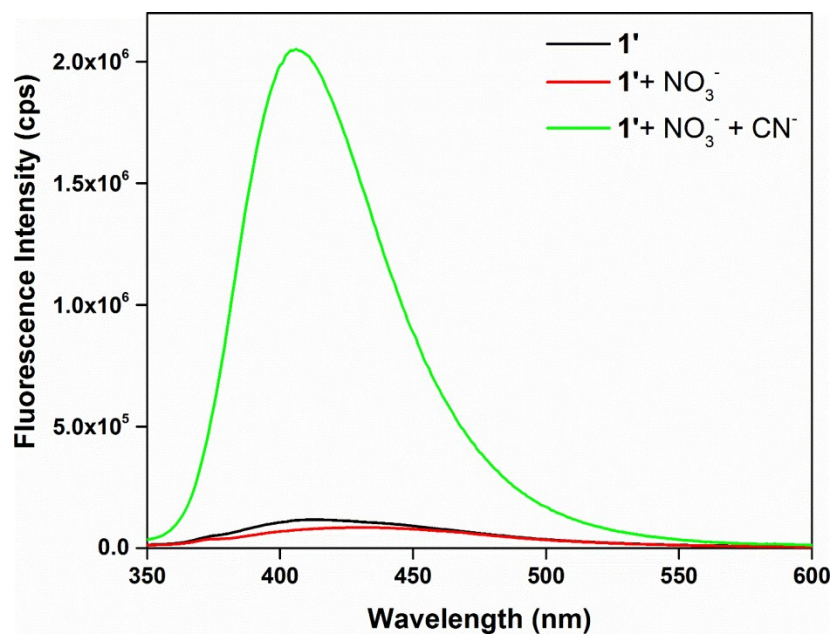


Figure S21. Change in the fluorescence intensity of **1'** upon addition of 4 mM CN⁻ solution (500 μL) in presence of NO₃⁻ ion (500 μL).

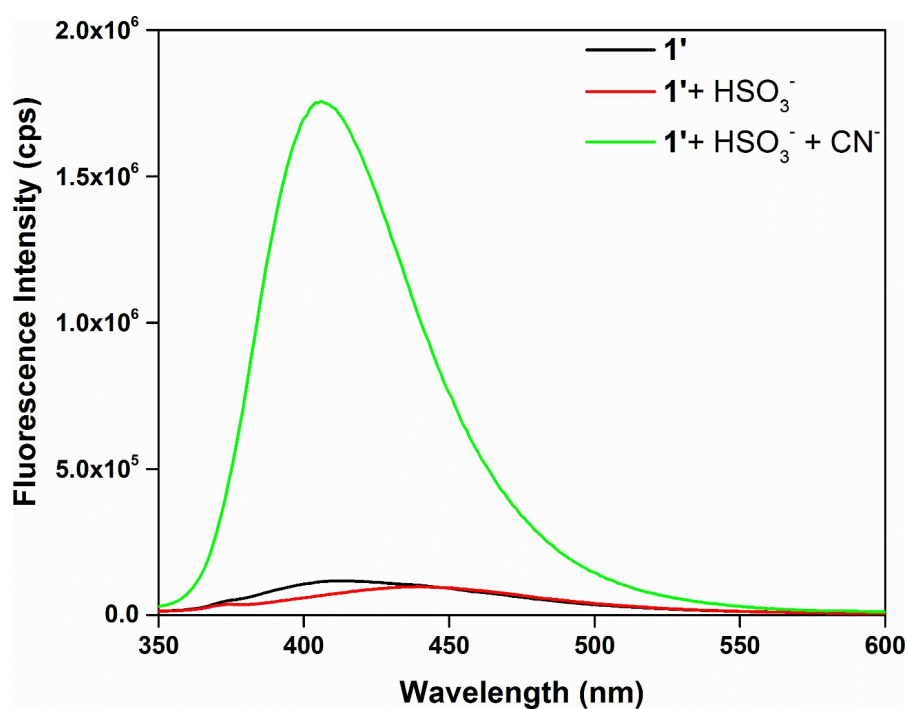


Figure S22. Change in the fluorescence intensity of **1'** upon addition of 4 mM CN^- solution (500 μL) in presence of HSO_3^- ion (500 μL).

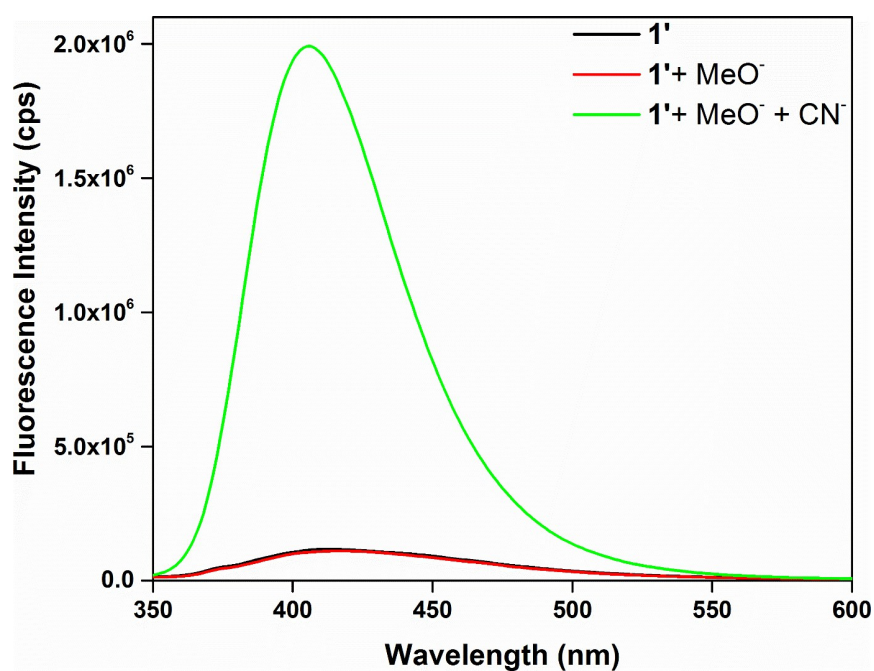


Figure S23. Change in the fluorescence intensity of **1'** upon addition of 4 mM CN^- solution (500 μL) in presence of HSO_3^- ion (500 μL).

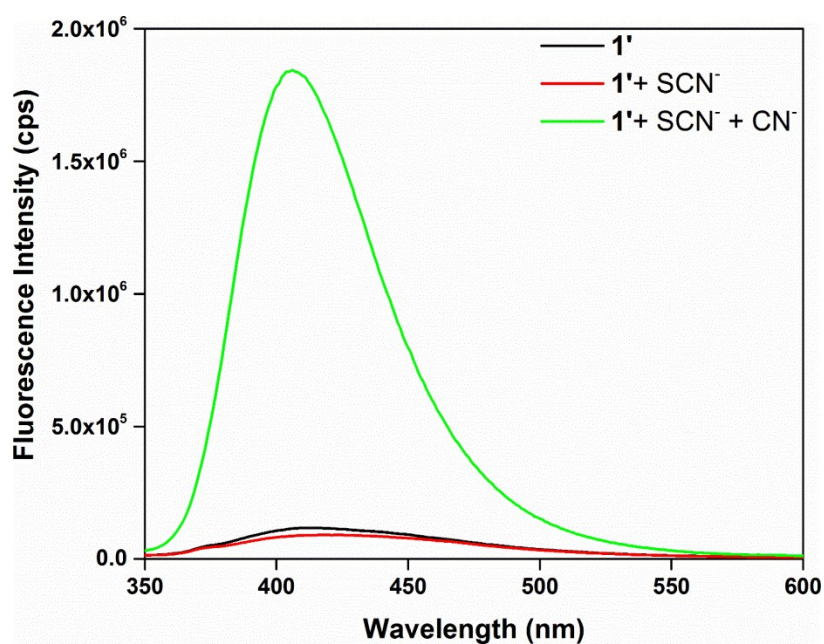


Figure S24. Change in the fluorescence intensity of **1'** upon addition of 4 mM CN^- solution (500 μL) in presence of SCN^- ion (500 μL).

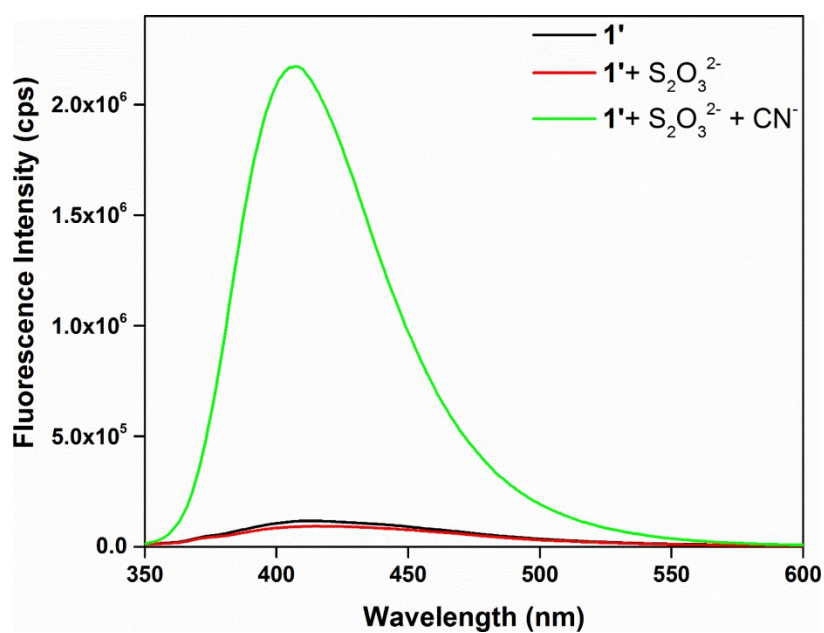


Figure S25. Change in the fluorescence intensity of **1'** upon addition of 4 mM CN^- solution (500 μL) in presence of $\text{S}_2\text{O}_3^{2-}$ ion (500 μL).

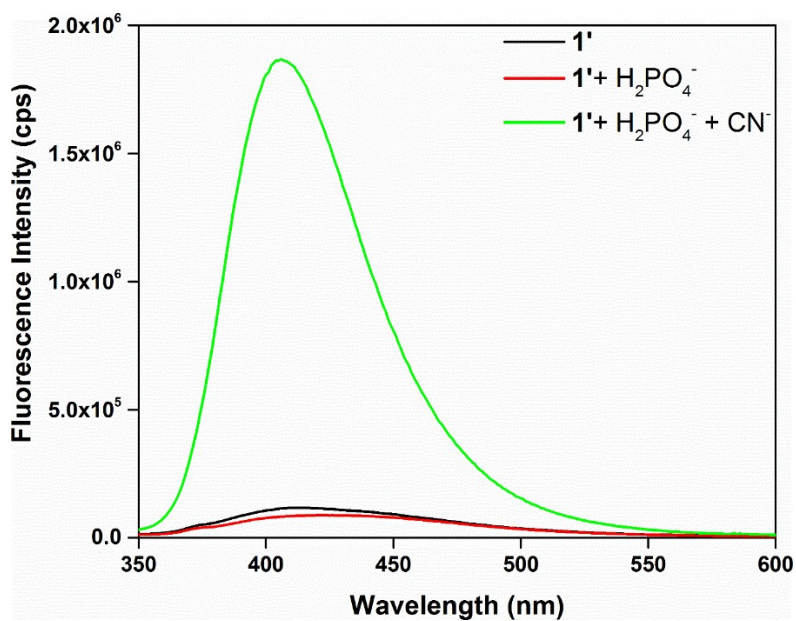


Figure S26. Change in the fluorescence intensity of **1'** upon addition of 4 mM CN^- solution (500 μL) in presence of H_2PO_4^- ion (500 μL).

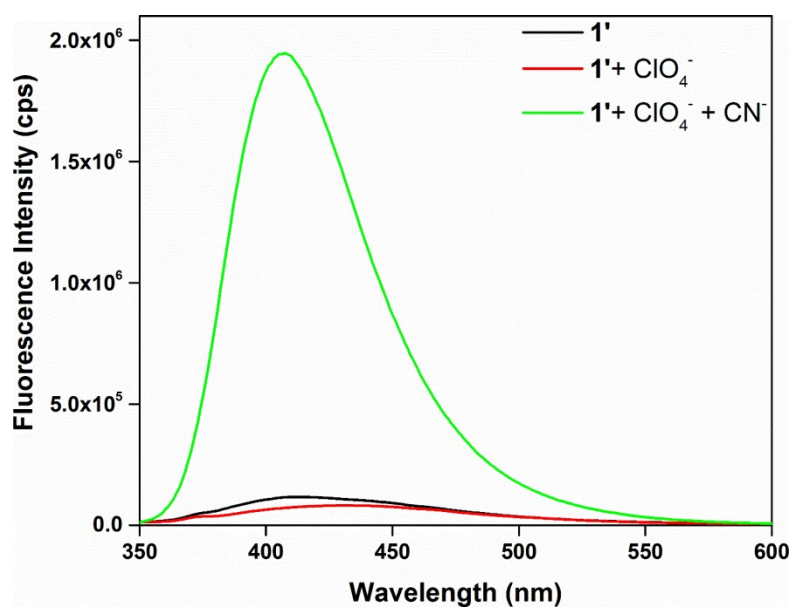


Figure S27. Change in the fluorescence intensity of **1'** upon addition of 4 mM CN^- solution (500 μL) in presence of ClO_4^- ion (500 μL).

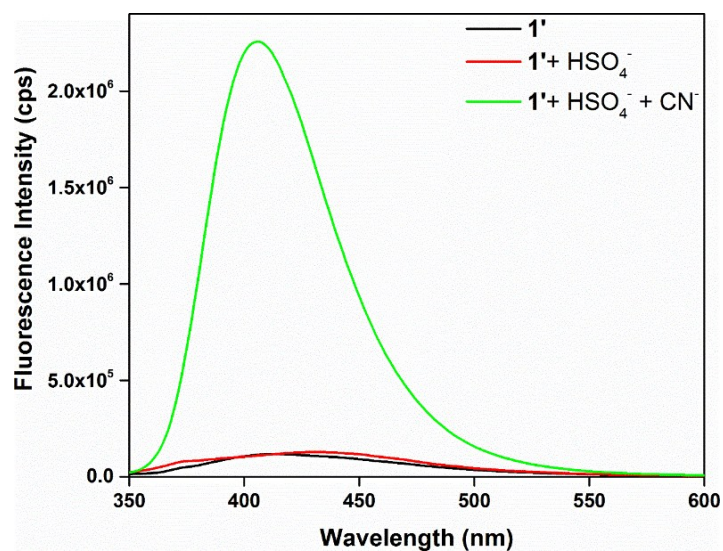


Figure S28. Change in the fluorescence intensity of **1'** upon addition of 4 mM CN^- solution (500 μL) in presence of HSO_4^- ion (500 μL).

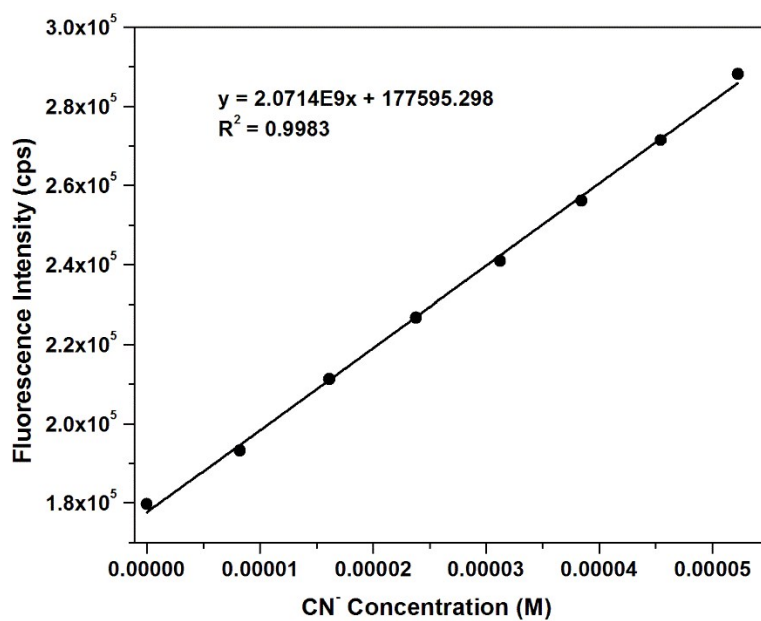


Figure S29. Change in the fluorescence intensity of **1'** in aqueous solution as a function of CN^- concentration.

Table S2. Comparison of the various existing fluorescent materials for the sensing of CN⁻.

Sl. No.	Sensor Material	Type of Material	Sensing Medium	Detection Limit	Ref.
1	CAU-10-N ₂ H ₃	MOF	Water	0.48 μM	This work
2	M-ZIF-90	MOF	DMSO/H ₂ O	2 μM	1
3	Carbazole-functionalized Zr(IV) MOF	MOF	Water	0.14 μM	2
4	Bio-MOF-1⊃DAAC	MOF	HEPES buffer	5.2 ppb	3
5	Tb-ADP-Bipy MOF	MOF	Water	30 nM	4
6	PAT-TFBE	Gel	Water	1.82 μM	5
7	BP	benzopyrylium–phenothiazine conjugate	CH ₃ CN/H ₂ O	0.13 μM	6
8	NBD-SSH–Cu ²⁺	peptide-based ensemble	Water	24.9 nM	7
9	Pyridyl azo-based chemosensors	Gel	Sol-gel medium	9.36 μM	8
10	pyridinium-fused pyridinone iodide	Chemodosimeter	THF/ H ₂ O	54 nM	9
11	3 T-2CN	Oligothiophene chemosensor	DMSO/H ₂ O	0.19 μM	10
12	AuAgNCs@ew	bimetallic gold–silver nanoclusters	Water	0.138 μM	11
13	{Ru ^{II} (^t Bubpy)(CN) ₄ –[Cu ^{II} (dien)] ₃ }(ClO ₄) ₂	trinuclear heterobimetallic Ru(II)–Cu(II) complex,	DMF/H ₂ O	1.2 μM	12
14	receptor 1	DMN conjugated benzothiazole	DMF/H ₂ O	0.16 μM	13
15	PNA⊃GBP·I ₂	supramolecular polymer	DMSO–H ₂ O	41 nM	14

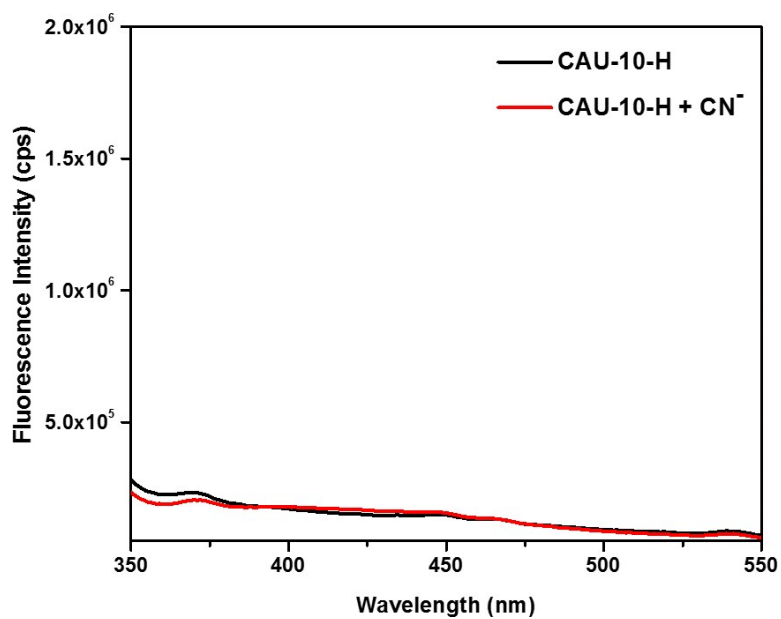


Figure S30. Change in the fluorescence intensity of CAU-10-H upon addition of 4 mM solution (500 μL) of aqueous CN^- solution.

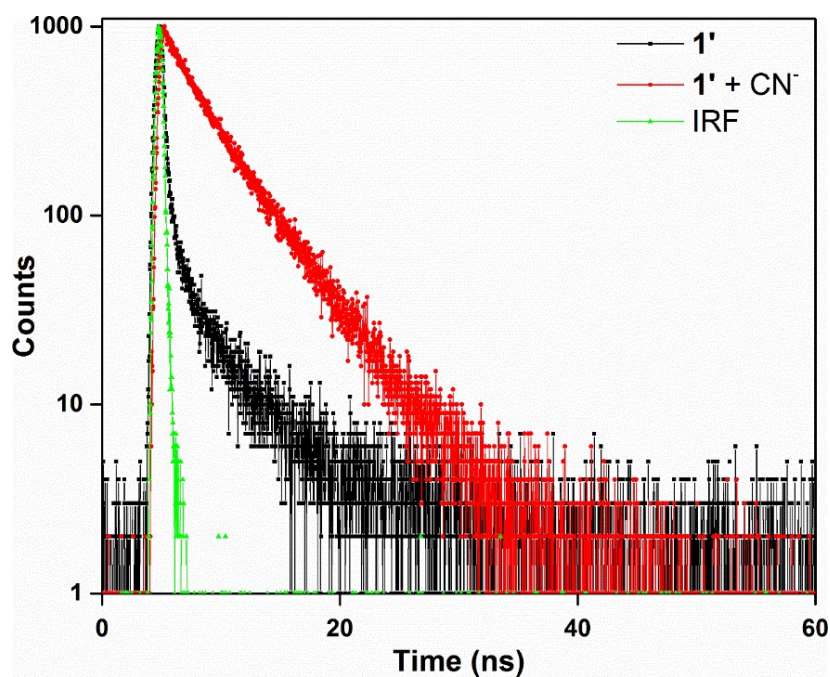


Figure S31. Lifetime decay profile of $1'$ in presence of aqueous CN^- solution ($\lambda_{\text{ex}} = 336 \text{ nm}$, monitored at 430 nm).

Table S3. Average excited-state lifetime ($\langle\tau\rangle$) values of **1'** before and after addition of CN⁻ solution ($\lambda_{\text{ex}} = 336 \text{ nm}$).

Volume of CN ⁻ solution added (μL)	a_1	a_2	τ_1 (ns)	τ_2 (ns)	$\langle\tau\rangle^*$ (ns)	χ^2
0	0.981	0.019	0.310	3.866	0.377	1.09
500	0.153	0.846	0.778	4.784	4.161	1.01

* $\langle\tau\rangle = a_1\tau_1 + a_2\tau_2$

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